Draft Risk Evaluation for 1,4-Dioxane
Draft Supplemental File:
Consumer Exposure Assessment
Model Input Parameters

November 2020

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Worksheet	Description
CEM Inputs - All Scenarios	This tab provides the model inputs required to evaluate the presented consumer conditions of use (COU) using EPA's Consumer Exposure Model (CEM 2.1).
MCCEM Inputs - SPF Scenarios	This tab provides the model inputs required to evaluate the inhalation pathway for the spray polyurethane foam (SPF) COU using EPA's Multi-Chamber Concentration and Exposure Model (MCCEM).
Weight Fractions	This tab provides the identified weight fractions and sources for all evaluated product scenarios.

Parameter	Units	Surface Cleaner	Antifreeze	Dish Soap
Chemical of Interest	n/a	1,4-Dioxane	1,4-Dioxane	1,4-Dioxane
CAS Number	n/a	123-91-1	123-91-1	123-91-1
CEM Model Scenario	n/a	Generic Product E1 (Emission from Product Applied to a Surface Indoors Incremental Source Model)	Generic Product E1 (Emission from Product Applied to a Surface Indoors Incremental Source Model)	Generic Product E4 (Emission from Product Added to Water)
Selected CEM Model Scenario - Dermal	n/a	Permeability (P_DER2b)	Absorption Fraction (P_DER2a)	Permeability (P_DER2b)
Product User (s)	n/a	Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)
Activity Pattern	n/a	User stays at home entire day	User stays at home entire day	User stays at home entire day
Product/Article Environment of Use	n/a	Bathroom	Garage	Kitchen
Background Concentration	mg/m^3	0	0	0
Select Pathways Evaluated in CEM	n/a	Inhalation and Dermal	Inhalation and Dermal	Inhalation and Dermal
Modeling Options - Inhalation	n/a	E1, Let CEM Estimate Emission Rate, P_INH2, Emission Factor Method	E1, Let CEM Estimate Emission Rate, P_INH2, Use Emission Factor Method	E4, Let CEM Estimate Emission Rate, P_INH2
Vapor Pressure (Lewis, 2010)	torr	40	40	40
Molecular Weight (Howard, 1990)	g/mol	88.1	88.1	88.1
Chemical Saturation Concentration in Air	mg/m^3	1.89E+05	1.89E+05	1.89E+05
Log Octanol-Water Partition Coefficient (Hansch et al., 1995)	n/a	-0.27	-0.27	-0.27
Water Solubility (Yalkowsky et al., 2010)	mg/mL	800	800	800
Gas Phase Mass Transfer Coefficient (CEM Estimate)	m/hr	3.2	3.2	3.2
Henry's Law Coefficient	atm/M	n/a	n/a	n/a
Emission Factor	$ug/m^2/hr$	0 (Chinn method)	0 (Chinn method)	n/a
Frequency of Use (Acute)	events/day	Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)
Frequency of Use (Chronic)	days/year	365 (CEM high-end default); 300 (CEM central-tendency default)	n/a [2]	365 (CEM high-end default); 300 (CEM central-tendency default)
Product Density	g/cm^3	1.09 (CEM scenario default)	1.12 (CEM scenario default)	1.03 (CEM scenario default)
Film Thickness on Skin	cm	0.00214 (CEM scenario default)	0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)	0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)
Product Dilution Factor	unitless	Fixed at 1 (i.e., no dilution)	Fixed at 1 (i.e., no dilution)	0.007 (estimated assuming high-end mass of product use [28g/use] in one gallon of water)
Maximum Weight Fraction	fraction	9.00E-06	8.60E-05	2.04E-04
Mean Weight Fraction	fraction	n/a (unable to estimate mean from available sources)	n/a [2]	2.40E-05
Duration of Use Event - High-End, Inhalation	min/events	30 (High-end scenario duration from CEM)	15 (High-end scenario duration from CEM)	20 (High-end scenario duration from CEM)
Duration of Use Event - Central Tendency, Inhalation	min/events	15 (Central tendency duration from Westat survey)	n/a [2]	10 (Central tendency scenario duration from CEM)
Duration of Use Event - High-End, Dermal	min/events	30 (High-end scenario duration from CEM)	15 (High-end scenario duration from CEM)	20 (High-end scenario duration from CEM)
Duration of Use Event - Central Tendency, Dermal	min/events	15 (Central tendency duration from Westat survey)	n/a [2]	10 (Central tendency scenario duration from CEM)
Mass Used - High-End	g/event	300 (High-end scenario duration from CEM)	150 (High-end scenario mass from CEM)	84 (High-end of range from American Cleaning Institute Exposure and Risk Screening Methods for Consumer Product Ingredients[6], which reported 28 g/use, up to three times per day)
Mass Used - Central Tendency	g/event	200 (Central tendency scenario duration from CEM)	n/a [2]	48 (Central tendency from American Cleaning Institute Exposure and Risk Screening Methods for Consumer Product Ingredients[6], with a mean of 16 g/use, up to three times per day)
Fraction Product Ingested	n/a	0.00E+00	0	0
Amount Retained on Skin	cm/hr	n/a	1.12E-4 (CEM Estimate)	n/a
Skin Permeability Coefficient (Kp)	cm/hr	5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)
Absorption Fraction High-End Dermal Duration	n/a	3.21E-01	2.62E-01 (CEM Estimate)	2.92E-01

Dishwasher Detergent	Laundry Detergent	Paint and Floor Lacquer	Textile Dye
1,4-Dioxane	1,4-Dioxane	1,4-Dioxane	1,4-Dioxane
123-91-1	123-91-1	123-91-1	123-91-1
Generic Product E4 (Emission from Product Added to Water)	Generic Product E4 (Emission from Product Added to Water)	Generic Product E2 (Emission from Product Applied to a Surface Indoors Double Exponential Model)	Generic Product E4 (Emission from Product Added to Water)
Absorption Fraction (P_DER2a)	Permeability (P_DER2b)	Absorption Fraction (P_DER2a)	Permeability (P_DER2b)
Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)
User stays at home entire day	User stays at home entire day	User stays at home entire day	User stays at home entire day
Kitchen	Utility Room	Bedroom	Utility Room
0	0	0	0
Inhalation and Dermal	Inhalation and Dermal	Inhalation and Dermal	Inhalation and Dermal
E4, Let CEM Estimate Emission Rate, P_INH2	E4, Let CEM Estimate Emission Rate, P_INH2	E2, Let CEM Estimate Emission Rate, P_INH2	E4, Let CEM Estimate Emission Rate, P_INH2
40	40	40	40
88.1	88.1	88.1	88.1
1.89E+05	1.89E+05	1.89E+05	1.89E+05
-0.27	-0.27	-0.27	-0.27
800	800	800	800
3.2	3.2	3.2	3.2
n/a	n/a	n/a	n/a
n/a	n/a	n/a	n/a
Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)
365 (CEM high-end default); 300 (CEM central-tendency default)	365 (CEM high-end default); 300 (CEM central-tendency default)	n/a [2]	n/a [2]
1.077 (CEM scenario default)	1.03 (CEM scenario default)	1.25 (CEM scenario default)	0.65 (CEM scenario default)
0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)	0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)	0.00981 (CEM scenario default)	0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)
Fixed at 1 (i.e., no dilution)	0.016 (estimated assuming high-end mass of product used [60g] in one gallon of water)	1 (i.e., no dilution)	0.1
9.70E-06	1.40E-05	3.00E-05	4.70E-06
5.00E-06	6.00E-06	n/a [2]	n/a [2]
50 (High-end scenario duration from CEM)	50 (High-end scenario duration from CEM)	810 (95th percentile duration from Westat survey	20 (High-end scenario duration from CEM)
45 (Central tendency scenario duration from CEM)	45 (Central tendency scenario duration from CEM)	n/a [2]	n/a [2]
1 [4]	20 (Central tendency scenario durations from CEM) [5]	810 (95th percentile duration from Westat survey	20 (High-end scenario duration from CEM)
1 [4]	10 (Central tendency scenario durations from CEM) [5]	n/a [2]	n/a [2]
40 (High-end scenario mass from CEM)	60 (High-end scenario mass from CEM)	26025 (95th percentile, Westat Survey)	100 (High-end scenario duration from CEM)
20 (Central tendency scenario mass from CEM)	40 (Central tendency mass from CEM)	n/a [2]	n/a [2]
0	0	0	0
1.08E-4 (CEM Estimate)	n/a	1.23E-2 (CEM Estimate)	n/a
5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)
3.77E-02	2.92E-01	3.38E-01	2.92E-01

SPF (Dermal)
1,4-Dioxane
123-91-1
n/a [1]
Absorption Fraction (P_DER2a)
Adult (Age ≥ 21) and Child (Age 11-20)
n/a [1]
n/a [1]
n/a [1]
Dermal
n/a [1]
40
88.1
1.89E+05
-0.27
800
3.2
n/a
n/a
Fixed at 1 event/day (CEM default)
n/a [2]
0.0384 (based on density of typical closed cell, medium density SPF, with densities ranging from 1.5 - 2.4 lbs/ft^3)
ACC, 2016
0.01 (CEM default)
1 (i.e., no dilution)
5.00E-04
n/a [2]
360 (basement, attic); 180 (garage)
n/a [2]
360 (basement, attic); 180 (garage)
n/a [2]
n/a [1]
n/a [2]
0
0.000384
5.05E-4 (IHSkinPerm)
3.38E-01

Absorption Fraction Central Tendency Dermal Duration [3]	n/a	2.62E-01	n/a [2]	2.14E-01
Surface Area-Body Weight (SA-BW) Adult	cm^2/kg	3.10 (CEM default mean, inside of one hand)	3.10 (CEM default mean, inside one hand)	12.4 (CEM default mean, both hands)
Surface Area-Body Weight (SA-BW) Adult 16-20	cm^2/kg	2.90 (CEM default mean, inside of one hand)	2.90 (CEM default mean, inside one hand)	11.6 (CEM default mean, both hands)
Surface Area-Body Weight (SA-BW) Child 11-15	cm^2/kg	3.17 (CEM default mean, inside of one hand)	3.17 (CEM default mean, inside one hand)	12.7 (CEM default mean, both hands)
Building Volume (Residence)	m^3	492	492	492
Use Environment Volume	m^3	15	90	24
Near Field/Far Field Volume	m^3	1/14	1/89	1/23
Air Exchange Rate, Zone 1 (Residence)	hr^{-1}	0.45 (CEM default)	0.45 (CEM default)	0.45 (CEM default)
Air Exchange Rate, Zone 2 (Residence)	hr^{-1}	0.45 (CEM default)	0.45 (CEM default)	0.45 (CEM default)
Interzone Ventilation Rate	m^3/hr	107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)
Air Exchange Rate, Near-Field Boundary	hr^{-1}	402 (CEM default)	402 (CEM default)	402 (CEM default)
Use Start Time	n/a	9:00 AM	9:00 AM	9:00 AM

[1] Inhalation exposures for the SPF scenario were evaluated using MCCEM with measured emission data, please see other tab for relevant inputs.

[2] Chronic exposures not evaluated for scenarios that are expected to involve infrequent and or intermittent use frequencies.

[3] For scenarios where chronic exposures are evaluated, central tendency durations of exposure were applied to dermal estimates, which impacts the estimation of absorption fraction within P_DER2a.

[4] The exposure duration applied for dermal exposures to dishwashing detergent were adjusted/lowered to 1 minute, as the scenario default exposure duration is based on the run time of a dishwasher, not on expected dermal contact time.

[5] The exposure duration applied for dermal exposures to laundry detergent were adjusted/lowered to be equal to the default exposures times for hand dish soap, as this dermal exposure scenario is intended to approximate dermal contact from hand washing of c

[6] https://www.aciscience.org/docs/Consumer_Product_Ingredient_Safety_v2.0.pdf

3.77E-02	2.14E-01	n/a [2]	n/a [2]
1.24 (CEM default mean, 10% of hands)	12.4 (CEM default mean, both hands)	15.8 (CEM default mean, face, hands, and arms)	12.4 (CEM default mean, both hands)
1.16 (CEM default mean, 10% of hands)	11.6 (CEM default mean, both hands)	14.9 (CEM default mean, face, hands, and arms)	11.6 (CEM default mean, both hands)
1.27 (CEM default mean, 10% of hands)	12.7 (CEM default mean, both hands)	16.4 (CEM default mean, face, hands, and arms)	12.7 (CEM default mean, both hands)
492	492	492	492
24	20	36	20
1/23	1/19	1/35	1/19
0.45 (CEM default)	0.45 (CEM default)	0.45 (CEM default)	0.45 (CEM default)
0.45 (CEM default)	0.45 (CEM default)	0.45 (CEM default)	0.45 (CEM default)
107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)
402 (CEM default)	402 (CEM default)	402 (CEM default)	402 (CEM default)
9:00 AM	9:00 AM	9:00 AM	9:00 AM

lothing, whereas the default exposure durations for the laundry detergent scenario are based on run times of the washing machine.

n/a [2]
15.8 (CEM default mean, face, hands, and arms)
14.9 (CEM default mean, face, hands, and arms)
16.4 (CEM default mean, face, hands, and arms)
n/a [1]
n/a [1]
n/a [1]
n/a [1]
n/a [1]
n/a [1]
n/a [1]
n/a [1]

Parameter	Units	Exposure Scenario		
		Attic	Basement	Garage
Model Start Time	day/hour/min	0/0/0	0/0/0	0/0/0
Length of Model Run	day/hour/min	10/0/0	10/0/0	10/0/0
Reporting Interval	day/hour/min	0/0/1	0/0/1	0/0/1
House Code	N/A	HY013	HY014	HY015
State	N/A	NA	NA	NA
Stories	N/A	2	2	2
Volume	m^3	615	492	610
Season	N/A	NA	NA	NA
Whole House ACH	1/hr	1.56	0.45	0.85
Number of Zones	N/A	2	2	2
Source Description	N/A	SPF	SPF	SPF
Start Time	day/hour/min	0/9/0	0/9/0	0/9/0
End Time	day/hour/min	0/15/0	0/15/0	0/12/0
Zone	N/A	1	1	1
Source Model	N/A	Incremental	Incremental	Incremental
Total Mass of Chemical Released	mg	4524	4528	2170
Percent of Mass Associated with First Exponential	%	100	100	100
First-Order Rate Constant (first exponential)	1/hour	0.1	0.1	0.1
First-Order Rate Constant (second exponential)	1/hour	0.1	0.1	0.1
Events per Year	1/year	0.1	0.1	0.1
Years of Exposure	years	57	57	57
Body Weight	kg	80	80	80
Length of Life	years	78	78	78

Attic Application Scenario

Zone Characteristics				
Zone Number	Description	Volume (m^3)	Total-Flow-In (m^3/hr)	Total-Flow-Out (m^3/hr)
1	Attic	123	799.50	799.50
2	ROH	492	282.90	282.90

Interzonal Air Flow Rate (m^3/hr)					
To From	Zone 0	Zone 1	Zone 2	Zone 3	Zone 4
Zone 0	-	738	221.4	0	0
Zone 1	738	-	61.5	0	0
Zone 2	221.4	61.5	-	0	0
Zone 3	0	0	0	-	0
Zone 4	0	0	0	0	-

Activity Pattern(s)				
Primary User Days in Effect: 1 Bystander Days in Effect: 0	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m^3/day)
	2	0	0	15.08
	1	9	0	15.08
	2	15	0	15.08
Secondary User Days in Effect: 2 - 7 Bystander Days in Effect: 1-7	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m^3/day)
	2	0	0	15.08

Basement Application Scenario

Zone Characteristics

Zone Number	Description	Volume (m³)	Total-Flow-In (m³/hr)	Total-Flow-Out (m³/hr)
1	Basement	246	219.70	219.70
2	ROH	246	219.70	219.70

Interzonal Air Flow Rate (m³/hr)					
To From	Zone 0	Zone 1	Zone 2	Zone 3	Zone 4
Zone 0	-	110.7	110.7	0	0
Zone 1	110.7	-	109	0	0
Zone 2	110.7	109	-	0	0
Zone 3	0	0	0	-	0
Zone 4	0	0	0	0	-

Activity Pattern(s)				
Primary User Days in Effect: 1 Bystander Days in Effect: 0	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08
	1	9	0	15.08
	2	15	0	15.08
Secondary User Days in Effect: 2 - 7 Bystander Days in Effect: 1-7	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08

Garage Application Scenario

Zone Characteristics				
Zone Number	Description	Volume (m³)	Total-Flow-In (m³/hr)	Total-Flow-Out (m³/hr)
1	Garage	118	404.00	404.00
2	ROH	492	330.40	330.40

Interzonal Air Flow Rate (m³/hr)					
To From	Zone 0	Zone 1	Zone 2	Zone 3	Zone 4
Zone 0	-	295	221.4	0	0
Zone 1	295	-	109	0	0
Zone 2	221.4	109	-	0	0
Zone 3	0	0	0	-	0
Zone 4	0	0	0	0	-

Activity Pattern(s)				
Primary User Days in Effect: 1 Bystander Days in Effect: 0	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08
	1	9	0	15.08
	2	12	0	15.08
Secondary User Days in Effect: 2 - 7 Bystander Days in Effect: 1-7	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08

Consumer Conditions of Use		Reported Product Concentrations (ppm)								
Category	**Subcategory**	Kwon et al., 2007	Fuh et al., 2005	Tanabe and Kawata, 2008	Tahara et al., 2013	OCA, 2009	Citizens Campaign for the Environment, 2018	Citizens Campaign for the Environment, 2019	ACA, 2015 Public Comment Submission (EPA-HQ-OPPT-2015-0078)	Sapphire Group Inc., 2007
Paints and Coatings	Paint or Floor Lacquer								0.02 - 30	
Cleaning and Furniture Care Products	Surface Cleaner	9		0.36 - 1.2						
Laundry and Dishwashing Products	Dish Soap				4.79 - 7.15	0.7 - 204		2.5 - 7.7		
Laundry and Dishwashing Products	Dishwasher Detergent		6.5	0.86 - 9.7						
Laundry and Dishwashing Products	Laundry Detergent			0.05 - 2.1			2 - 14	0.22 - 14		
Arts, Crafts, and Hobby Materials	Textile Dye									
Other Consumer Uses	Spray Polyurethane Foam	*Based on concentration of mixed SPF used in the occupational expo*								
Automotive Care Products	Antifreeze									0.01 - 22

[1] The select Safety Data Sheet may now be superseded by a more recent version or formulation.

Makino et al., 2006	Danish EPA, 2005	Peak Extended Life Antifreeze & Coolant (2002) Safety Data Sheet1	**Overall Range (ppm)**	**Mean (ppm)**	**Maximum Weight Fraction (%)**	**Maximum Weight Fraction Input**	**Mean Weight Fraction Input**
			0.02 - 30		0.003%	3.00E-05	
			0.36 - 9	Cannot estimate - unknown number of products tested in Kwon et al., 2007	0.0009%	9.00E-06	n/a
51			0.7 - 204	24	0.0204%	2.04E-04	2.40E-05
			0.86 - 9.7	5	0.00097%	9.70E-06	5.00E-06
< 25			0.05 - 14	6	0.0014%	1.40E-05	6.00E-06
	4.7		4.7		0.00047%	4.70E-06	
sure scenario					0.05%	5.00E-04	
		86	0.01 - 86		0.0086%	8.60E-05	